Working with NumPy Arrays

NumPy, or Numerical Python, is a Python-based library for mathematical computations and processing arrays. Python does not support data structures in more than one dimension, with containers like lists, tuples, and dictionaries being unidimensional. The inbuilt data types and containers in Python cannot be restructured into more than one dimension, and also do not lend themselves to complex computations. These drawbacks are limitations for some of the tasks involved while analyzing data and building models, which makes arrays a vital data structure.

NumPy arrays can be reshaped and utilize the principle of vectorization (where an operation applied to the array reflects on all its elements).

In the previous chapter, we looked at the basic concepts used in descriptive data analysis. NumPy is an integral part of many of the tasks we perform in data analysis, serving as the backbone of many of the functions and data types used in Pandas. In this chapter, we understand how to create NumPy arrays using a variety of methods, combine arrays, and slice, reshape, and perform computations on them.

Getting familiar with arrays and NumPy functions

Here, we look at various methods of creating and combining arrays, along with commonly used NumPy functions.

Importing the NumPy package

The NumPy package has to be imported before its functions can be used, as shown in the following. The shorthand notation or alias for NumPy is np.

CODE:

import numpy as np

If you have not already installed NumPy, go to the Anaconda Prompt and enter the following command:

pip install numpy

Creating an array

The basic unit in NumPy is an array. In Table 5-1, we look at the various methods for creating an array.

Table 5-1. Methods of Creating NumPy Arrays

Method	Example
Creating an array from a list	The <i>np.array</i> function is used to create a one-dimensional or multidimensional array from a list.
	CODE: np.array([[1,2,3],[4,5,6]])
	Output: array([[1, 2, 3],
Creating an array from a range	The np.arange function is used to create a range of integers. CODE: np.arange(0,9) #Alternate syntax: np.arange(9) #Generates 9 equally spaced integers starting from 0 Output: array([0, 1, 2, 3, 4, 5, 6, 7, 8])
Creating an array of equally spaced numbers	The <i>np.linspace</i> function creates a given number of equally spaced values between two limits. CODE: np.linspace(1,6,5) # This generates five equally spaced values between 1 and 6
	Output: array([1. , 2.25, 3.5 , 4.75, 6.])

(continued)

Table 5-1. (continued)

Method **Example** Creating an array The *np.zeros* function creates an array with a given number of rows and of zeros columns, with only one value throughout the array – "0". CODE: np.zeros((4,2))#Creates a 4*2 array with all values as 0 Output: array([[0., 0.], [0., 0.],[0., 0.], [0., 0.]]) The *np.ones* function is similar to the *np.zeros* function, the difference being Creating an array of ones that the value repeated throughout the array is "1". CODE: np.ones((2,3))#creates a 2*3 array with all values as 1 Output: array([[1., 1., 1.], [1., 1., 1.]]) Creating an array The *np.full* function creates an array using the value specified by the user. with a given CODE: value repeated np.full((2,2),3)throughout #Creates a 2*2 array with all values as 3 Output: array([[3, 3], [3, 3]])

(continued)

Table 5-1. (continued)

Method	Example
Creating an empty array	The <i>np.empty</i> function generates an array, without any particular initial value (array is randomly initialized).
	CODE: np.empty((2,2)) #creates a 2*2 array filled with random values
	Output: array([[1.31456805e-311, 9.34839993e+025],
Creating an array from a repeating list	The <i>np.repeat</i> function creates an array from a list that is repeated a given number of times.
	<pre>CODE: np.repeat([1,2,3],3) #Will repeat each value in the list 3 times</pre>
	Output: array([1, 1, 1, 2, 2, 2, 3, 3, 3])
Creating an array of random integers	The <i>randint</i> function (from the <i>np.random</i> module) generates an array containing random numbers.
	CODE: np.random.randint(1,100,5) #Will generate an array with 5 random numbers between 1 and 100
	Output: array([34, 69, 67, 3, 96])

One point to note is that arrays are homogeneous data structures, unlike containers (like lists, tuples, and dictionaries); that is, an array should contain items of the same data type. For example, we cannot have an array containing integers, strings, and floating-point (decimal) values together. While defining a NumPy array with items of different data types does not lead to an error while you write code, it should be avoided.

Now that we have looked at the various ways of defining an array, we look at the operations that we can perform on them, starting with the reshaping of an array.

Reshaping an array

Reshaping an array is the process of changing the dimensionality of an array. The NumPy method "reshape" is important and is commonly used to convert a 1-D array to a multidimensional one.

Consider a simple 1-D array containing ten elements, as shown in the following statement.

```
CODE:

x=np.arange(0,10)

Output:

array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

We can reshape the 1-D array "x" into a 2-D array with five rows and two columns:

```
CODE:
```

x.reshape(5,2)

As another example, consider the following array:

```
CODE:
```

```
x=np.arange(0,12)
x
Output:
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
```

Now, apply the *reshape* method to create two subarrays - each with three rows and two columns:

```
CODE:
```

The product of the dimensions of the reshaped array should equal the number of elements in the original array. In this case, the dimensions of the array (2,3,2) when multiplied equal 12, the number of elements in the array. If this condition is not satisfied, reshaping fails to work.

Apart from the *reshape* method, we can also use the *shape* attribute to change the shape or dimensions of an array:

CODE:

```
x.shape=(5,2)
#5 is the number of rows, 2 is the number of columns
```

Note that the *shape* attribute makes changes to the original array, while the *reshape* method does not alter the array.

The reshaping process can be reversed using the "ravel" method:

```
x=np.arange(0,12).reshape(2,3,2)
x.ravel()
Output:
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11])
122
```

Further reading: See more on array creation routines: https://numpy.org/doc/stable/reference/routines.array-creation.html#

The logical structure of arrays

The cartesian coordinate system, which is used to specify the location of a point, consists of a plane with two perpendicular lines known as the "x" and "y" axes. The position of a point is specified using its x and y coordinates. This principle of using axes to represent different dimensions is also used in arrays.

A 1-D array has one axis (axis=0) as it has one dimension, as shown in Figure 5-1.



Figure 5-1. 1-D array representation

A 2-D array has an axis value of "0" to represent the row axis and a value of "1" to represent the column axis, as shown in Figure 5-2.

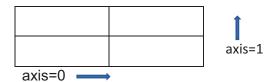


Figure 5-2. A 2-D array representation

A 3-D array has three axes, representing three dimensions, as shown in Figure 5-3.

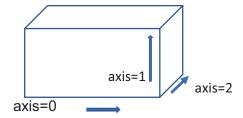


Figure 5-3. A 3-D array representation

Extending the logic, an array with "n" dimensions has "n" axes.

Note that the preceding diagrams represent only the logical structure of arrays. When it comes to storage in the memory, elements in an array occupy contiguous locations, regardless of the dimensions.

Data type of a NumPy array

The *type* function can be used to determine the type of a NumPy array:

CODE:

```
type(np.array([1,2,3,4]))
```

Output:

numpy.ndarray

Modifying arrays

The length of an array is set when you define it. Let us consider the following array, "a":

CODE:

```
a=np.array([0,1,2])
```

The preceding code statement would create an array of length 3. The array length is not modifiable after this. In other words, we cannot add a new element to the array after its definition.

The following statement, where we try to add a fourth element to this array, would lead to an error:

CODE:

a[3]=4

Output:

```
IndexErrorTraceback (most recent call last)
<ipython-input-215-94b083a55c38> in <module>
---> 1a[3]=4
```

IndexError: index 3 is out of bounds for axis 0 with size 3

However, you can change the value of an existing element. The following statement would work fine:

CODE:

In summary, while you can modify the values of existing items in an array, you cannot add new items to it.

Now that we have seen how to define and reshape an array, we look at the ways in which we can combine arrays.

Combining arrays

There are three methods for combining arrays: appending, concatenation, and stacking.

1. **Appending** involves joining one array at the end of another array. The *np.append* function is used to append two arrays.

```
CODE:
```

```
x=np.array([[1,2],[3,4]])
y=np.array([[6,7,8],[9,10,11]])
np.append(x,y)
Output:
array([ 1,  2,  3,  4,  6,  7,  8,  9, 10, 11])
```

2. **Concatenation** involves joining arrays along an axis (either vertical or horizontal). The *np.concatenate* function concatenates arrays.

```
CODE:
```

```
x=np.array([[1,2],[3,4]])
y=np.array([[6,7],[9,10]])
np.concatenate((x,y))
```

Output:

By default, the *concatenate* function joins the arrays vertically (along the "0" axis). If you want the arrays to be joined side by side, the "axis" parameter needs to be added with the value as "1":

CODE:

```
np.concatenate((x,y),axis=1)
```

The *append* function uses the *concatenate* function internally.

3. **Stacking**: Stacking can be of two types, vertical or horizontal, as explained in the following.

Vertical stacking

As the name indicates, vertical stacking stacks arrays one below the other. The number of elements in each subarray of the arrays being stacked vertically must be the same for vertical stacking to work. The *np.vstack* function is used for vertical stacking.

```
x=np.array([[1,2],[3,4]])
y=np.array([[6,7],[8,9],[10,11]])
np.vstack((x,y))

Output:
array([[1, 2],
        [3, 4],
        [6, 7],
        [8, 9],
        [10, 11]])
```

See how there are two elements in each subarray of the arrays "x" and "y".

Horizontal stacking

Horizontal stacking stacks arrays side by side. The number of subarrays needs to be the same for each of the arrays being horizontally stacked. The *np.hstack* function is used for horizontal stacking.

In the following example, we have two subarrays in each of the arrays, "x" and "y".

```
CODE:
```

```
x=np.array([[1,2],[3,4]])
y=np.array([[6,7,8],[9,10,11]])
np.hstack((x,y))

Output:
array([[ 1,  2,  6,  7,  8],
        [ 3,  4,  9,  10,  11]])
```

In the next section, we look at how to use logical operators to test for conditions in NumPy arrays.

Testing for conditions

NumPy uses logical operators $(\&,|,\sim)$, and functions like np.any, np.all, and np.where to check for conditions. The elements in the array (or their indexes) that satisfy the condition are returned.

Consider the following array:

```
CODE:
```

```
x=np.linspace(1,50,10)
x
```

```
Output:
```

```
array([ 1. , 6.44444444, 11.88888889, 17.33333333, 22.77777778, 28.22222222, 33.66666667, 39.11111111, 44.55555556, 50. ])
```

Let us check for the following conditions and see which elements satisfy them:

• Checking if all the values satisfy a given condition: The *np.all* function returns the value "True" only if the condition holds for all the items of the array, as shown in the following example.

CODE:

```
np.all(x>20)
#returns True only if all the elements are greater than 20
```

Output:

False

• Checking if any of the values in the array satisfy a condition: The *np. any* function returns the value "True" if any of the items satisfy the condition.

CODE:

```
np.any(x>20)
#returns True if any one element in the array is greater than 20
Output:
```

True

• Returning the index of the items satisfy a condition: The *np.where* function returns the index of the values in the array satisfying a given condition.

```
CODE:
```

```
np.where(x<10)
#returns the index of elements that are less than 10</pre>
```

Output:

```
(array([0, 1], dtype=int64),)
```

The *np.where* function is also useful for selectively retrieving or filtering values in an array. For example, we can retrieve those items that satisfy the condition "x<10", using the following code statement:

CODE:

```
x[np.where(x<10)]
Output:
```

```
array([1. , 6.4444444])
```

• Checking for more than one condition:

NumPy uses the following Boolean operators to combine conditions:

• & operator (equivalent to *and* operator in Python): Returns True when all conditions are satisfied:

CODE:

```
x[(x>10) & (x<50)]
```

#Returns all items that have a value greater than 10 and less than 50

Output:

```
array([11.88888889, 17.33333333, 22.77777778, 28.22222222, 33.66666667, 39.11111111, 44.55555556])
```

• | operator (equivalent to *or* operator in Python): Returns True when any one condition, from a given set of conditions, is satisfied.

```
x[(x>10) \mid (x<5)] #Returns all items that have a value greater than 10 or less than 5
```

```
Output:
```

```
array([ 1. , 11.88888889, 17.33333333, 22.77777778, 28.2222222, 33.66666667, 39.11111111, 44.55555556, 50. ])
```

~ operator (equivalent to *not* operator in Python) for negating a condition.

```
CODE:
```

```
x[~(x<8)]
#Returns all items greater than 8
Output:
array([11.88888889, 17.33333333, 22.77777778, 28.22222222, 33.66666667, 39.11111111, 44.55555556, 50. ])</pre>
```

We now move on to some other important concepts in NumPy like broadcasting and vectorization. We also discuss the use of arithmetic operators with NumPy arrays.

Broadcasting, vectorization, and arithmetic operations

Broadcasting

When we say that two arrays can be broadcast together, this means that their dimensions are compatible for performing arithmetic operations on them. Arrays can be combined using arithmetic operators as long as the rules of broadcasting are followed, which are explained in the following.

1. Both the arrays have the same dimensions.

In this example, both arrays have the dimensions 2*6.

```
x=np.arange(0,12).reshape(2,6)
y=np.arange(5,17).reshape(2,6)
x*y
```

Output:

```
array([[ 0, 6, 14, 24, 36, 50], [ 66, 84, 104, 126, 150, 176]])
```

2. One of the arrays is a one-element array.

In this example, the second array has only one element.

CODE:

```
x=np.arange(0,12).reshape(2,6)
y=np.array([1])
x-y
Output:
array([[-1, 0, 1, 2, 3, 4],
[ 5, 6, 7, 8, 9, 10]])
```

3. An array and a scalar (a single value) are combined.

In this example, the variable y is used as a scalar value in the operation.

CODE:

```
x=np.arange(0,12).reshape(2,6)
y=2
x/y
Output:
array([[0., 0.5, 1., 1.5, 2., 2.5],
[3., 3.5, 4., 4.5, 5., 5.5]])
```

We can add, subtract, multiply, and divide arrays using either the arithmetic operators (+/-/* and /), or the functions (*np.add*, *np.subtract*, *np.multiply*, and *np.divide*)

```
np.add(x,y)
#Or
x+y
```

Output:

```
array([[ 6, 8], [11, 13]])
```

Similarly, you can use *np.subtract* (or the – operator) for subtraction, *np.multiply* (or the * operator) for multiplication, and *np.divide* (or the / operator) for division.

Further reading: See more on array broadcasting: https://numpy.org/doc/stable/user/basics.broadcasting.html

Vectorization

Using the principle of vectorization, you can also conveniently apply arithmetic operators on each object in the array, instead of iterating through the elements, which is what you would do for applying operations to items in a container like a list.

CODE:

```
x=np.array([2,4,6,8])
x/2
#divides each element by 2
Output:
array([1., 2., 3., 4.])
```

Dot product

We can obtain the dot product of two arrays, which is different from multiplying two arrays. Multiplying two arrays gives an element-wise product, while a dot product of two arrays computes the inner product of the elements.

If we take two arrays,

|PQ| |RS| and |UV|

|WX|

The dot product is given by

$$|PQ|$$
 . $|UV|$ = $|P*U+Q*VP*V+Q*X|$
 $|RS|$ $|WX|$ $|R*U+S*WR*V+S*X|$

Multiplying the arrays gives the following result:

$$|PQ| * |UV| = |P*U Q*V|$$

 $|R S| |WX| |R*WS*X|$

As discussed earlier, arrays can be multiplied using the multiplication operator (*) or the np.multiply function.

The NumPy function for obtaining the dot product is *np.dot*.

CODE:

```
np.dot(x,y)
Output:
```

We can also combine an array with a scalar.

In the next topic, we discuss how to obtain the various properties or attributes of an array.

Obtaining the properties of an array

Array properties like their size, dimensions, number of elements, and memory usage can be found out using attributes.

Consider the following array:

```
x=np.arange(0,10).reshape(5,2)
```

• The *size* property gives the number of elements in the array.

CODE:

x.size

```
Output:
10
The ndim property gives the number of dimensions.
CODE:
x.ndim
Output:
2
The memory (total number of bytes) occupied by an array can be
calculated using the nbytes attribute.
CODE:
x.nbytes
Output:
40
Each element occupies 4 bytes (since this is an int array);
therefore, ten elements occupy 40 bytes
The data type of elements in this array can be calculated using the
dtype attribute.
CODE:
x.dtype
Output:
dtype('int32')
```

Note the difference between the *dtype* and the *type* of an array. The *type* function gives the type of the container object (in this case, the type is *ndarray*), and dtype, which is an attribute, gives the type of individual items in the array.

Further reading: Learn more about the list of data types supported by NumPy: https://numpy.org/devdocs/user/basics.types.html

Transposing an array

The transpose of an array is its mirror image.

Consider the following array:

CODE:

```
x=np.arange(0,10).reshape(5,2)
```

There are two methods for transposing an array:

• We can use the *np.transpose* method.

CODE:

```
np.transpose(x)
```

• Alternatively, we can use the T attribute to obtain the transpose.

CODE:

x.T

Both methods give the same output:

```
array([[0, 2, 4, 6, 8], [1, 3, 5, 7, 9]])
```

Masked arrays

Let us say that you are using a NumPy array to store the scores obtained in an exam for a class of students. While you have data for most students, there are some missing values. A masked array, which is used for storing data with invalid or missing entries, is useful in such scenarios.

A masked array can be defined by creating an object of the "ma.masked_array" class (part of the numpy.ma module):

```
import numpy.ma as ma
x=ma.masked_array([87,99,100,76,0],[0,0,0,0,1])
#The last element is invalid or masked
x[4]
```

Output:

Masked

Two arrays are passed as arguments to the *ma.masked_array* class – one containing the values of the items in the array, and one containing the mask values. A mask value of "0" indicates that the corresponding item value is valid, and a mask value of "1" indicates that it is missing or invalid. For instance, in the preceding example, the values 87, 99, 100, and 76 are valid since they have a mask value of "0". The last item in the first array (0), with a mask value of "1", is invalid.

The mask values can also be defined using the mask attribute.

CODE:

```
x=ma.array([87,99,100,76,0])
x.mask=[0,0,0,0,1]
```

To unmask an element, assign it a value:

CODE:

x[4]=82

The mask value for this element changes to 1 since it is no longer invalid.

Let us now look at how to create subsets from an array.

Slicing or selecting a subset of data

Slicing of arrays is similar to the slicing of strings and lists in Python. A slice is a subset of a data structure (in this case, an array), which can represent a set of values or a single value.

Consider the following array:

```
x=np.arange(0,10).reshape(5,2)
```

```
Output:
```

Some examples of slicing are given in the following.

• Select the first subarray [0,1]:

CODE:

x[0]

Output:

```
array([0, 1])
```

• Select the second column:

```
CODE:
```

```
x[:,1] #This will select all the rows and the 2^{nd}column (has an index of 1)
```

Output:

```
array([1, 3, 5, 7, 9])
```

• Select the element at the fourth row and first column:

CODE:

x[3,0]

Output:

6

• We can also create a slice based on a condition:

CODE:

x[x<5]

Output:

When we slice an array, the original array is not modified (a copy of the array is created).

Now that we have learned about creating and working with arrays, we move on to another important application of NumPy – calculation of statistical measures using various functions.

Obtaining descriptive statistics/aggregate measures

There are methods in NumPy that enable simplification of complex calculations and determination of aggregate measures.

Let us find the measures of central tendency (the mean, variance, standard deviation), sum, cumulative sum, and the maximum value for this array:

```
CODE:
```

```
x=np.arange(0,10).reshape(5,2)
#mean
x.mean()
```

Output:

4.5

Finding out the variance:

CODE:

x.var() #variance

Output:

2.91666666666665

Calculating the standard deviation:

CODE:

x.std() #standard deviation

Output:

1.707825127659933

Calculating the sum for each column:

CODE:

x.sum(axis=0) #calculates the column-wise sum

Output:

array([6, 15])

Calculating the cumulative sum:

CODE:

x.cumsum()

#calculates the sum of 2 elements at a time and adds this sum to the next element

Output:

Finding out the maximum value in an array:

CODE:

x.max()

Output:

9

Before concluding the chapter, let us learn about matrices – another data structure supported by the NumPy package.

Matrices

A matrix is a two-dimensional data structure, while an array can consist of any number of dimensions.

With the *np.matrix* class, we can create a matrix object, using the following syntax:

CODE:

```
x=np.matrix([[2,3],[33,3],[4,1]])
#OR
x=np.matrix('2,3;33,3;4,1') #Using semicolons to separate the rows
x
Output:
matrix([[2,3],[33,3],[4,1]])
[33, 3],
[4, 1]])
```

Most of the functions that can be applied to arrays can be used on matrices as well. Matrices use some arithmetic operators that make matrix operations more intuitive. For instance, we can use the * operator to get the dot product of two matrices that replicates the functionality of the *np.dot* function.

Since matrices are just one specific case of arrays and might be deprecated in future releases of NumPy, it is generally preferable to use NumPy arrays.

Summary

- NumPy is a library used for mathematical computations and creating data structures, called arrays, that can contain any number of dimensions.
- There are multiple ways for creating an array, and arrays can also be reshaped to add more dimensions or change the existing dimensions.

- Arrays support vectorization that provides a quick and intuitive method to apply arithmetic operators on all the elements of the array.
- A variety of statistical and aggregate measures can be calculated using simple NumPy functions, like np.mean, np.var, np.std, and so on.

Review Exercises

Question 1

Create the following array:

Slice the preceding array to obtain the following:

- Elements in the third subarray (17,18,19,20,21,22,23,24)
- Last element (24)
- Elements in the second column (2,6,10,14,18,22)
- Elements along the diagonal (1,10,19,24)

Question 2

Use the appropriate NumPy function for creating each of these arrays:

- An array with seven random numbers
- An uninitialized 2*5 array
- An array with ten equally spaced floating-point numbers between 1 and 3
- A 3*3 array with all the values as 100

Question 3

Write simple code statements for each of the following:

- Create an array to store the first 50 even numbers
- Calculate the mean and standard deviation of these numbers
- Reshape this array into an array with two subarrays, each with five rows and five columns
- Calculate the dimensions of this reshaped array

Question 4

Compute the dot product of these two data structures:

```
[[ 2, 3],
[33, 3],
[ 4, 1]]
AND
[[ 2, 3, 33],
[ 3, 4, 1]]
```

Using

- 1. Matrices
- 2. Arrays

Question 5

What is the difference between the code written in parts 1 and 2, and how would the outputs differ?

```
Part 1:
CODE:
x=np.array([1,2,3])
x*3
```

Part 2: CODE:

a=[1,2,3] a*3

Answers

Question 1

x=np.arange(1,25).reshape(3,2,4)

• Elements in the third subarray (17,18,19,20,21,22,23,24):

CODE:

x[2]

• Last element (24):

CODE:

x[2,1,3]

• Elements in the second column (2,6,10,14,18,22):

CODE:

x[:,:,1]

• Elements along the diagonal (1,10,19,24):

CODE:

Question 2

• An array with seven random numbers:

CODE:

np.random.randn(7)

• An uninitialized 2*5 array:

```
CODE: np.empty((2,5))
```

• An array with ten equally spaced floating-point numbers between 1 and 3:

```
CODE:
np.linspace(1,3,10)
```

• A 3*3 array with all the values as 100:

```
CODE: np.full((3,3),100)
```

Question 3

CODE:

```
#creating the array of first 50 even numbers
x=np.arange(2,101,2)
#calculating the mean
x.mean()
#calculating the standard deviation
x.std()
#reshaping the array
y=x.reshape(2,5,5)
#calculating its new dimensions
y.ndim
```

Question 4

Computing the dot product using matrices requires the use of the * arithmetic operator

```
x=np.matrix([[2,3],[33,3],[4,1]])
y=np.matrix([[2,3,33],[3,4,1]])
x*y
```

Computing the dot product using arrays requires the use of the dot method.

CODE:

```
x=np.array([[2,3],[33,3],[4,1]])
y=np.array([[2,3,33],[3,4,1]])
x.dot(y)
```

Question 5

Outputs:

1. array([3, 6, 9])

An array supports vectorization, and thus the * operator is applied to each element.

2. [1, 2, 3, 1, 2, 3, 1, 2, 3]

For a list, vectorization is not supported, and applying the * operator simply repeats the list instead of multiplying the elements by a given number. A "for" loop is required to apply an arithmetic operator on each item.